or when the computer system was engaged in developmental work. For example, to build the library of low resolution mass spectral data of sterols, several LRMS of new compounds were obtained by GC/MS. Also, in collaboration with Dr. Meflin, Dept. of Cardiology, we have investigated the use of specific ion monitoring as a tool for the identification of a new drug and its primary metabolite in human serum. Spectra of porphyrins have been obtained for Dr. Collman's group, Dept. of Chemistry, in studies of model systems for oxygen transport. We have obtained spectra of heart beat stimulants (digitoxigenins) for Prof. Kalman in Pharmacology, to verify identities of these compounds.

3.4 Applications of Programs by External Scientists

The DENDRAL project, one of the major users of the SUMEX-AIM computer facility, has formed a small community of regular, remote users. This "exodendral" community has continued to provide valuable contributions to program development, although the growth of this community has had to be slowed in response to increasing demands by other projects upon the SUMEX-AIM facility. As an example, for the months of September 1975 to February 1976, the number of CPU hours used by exodendral persons amounted to at least 8 percent of the CPU hours used by the DENDRAL project. There are currently four remote chemist-users whose groups regularly use CONGEN in their day to day work. Additionally, there are several remote users who use their accounts on an occasional basis, or who access SUMEX-AIM via the GUEST mechanism.

The SUMEX-AIM facility has grown markedly in number of projects over the past year. Due to this increase in system loading; the DENDRAL project, which had previously been able to offer trial usage of its programs to almost any chemist who expressed a need to use the programs, has found itself in the unfortunate position of of having to carefully screen potential collaborators. Those chemists who have been granted access, have been requested to restrict their usage to off-prime time hours. CONGEN, the DENDRAL program which receives most of this usage, has evolved in a manner designed to try to remedy the system loading problem which can be created by the enthusiasm of it's chemist-users. Since a typical, long GENERATE, PRUNE or IMBED within CONGEN can be very time consuming, as well as a voracious consumer of CPU cycles, a provision to permit a user to easily take advantage of SUMEX-AIM's off-hour batch processing has been implemented. A CONGEN user can now interactively set up his problem, and when ready to commence with a time consuming procedure, can, from within CONGEN, request automatic submission to BATCH, to be run late at night. The CONGEN users also benefit from this ability, in that they no longer must leave a terminal tied up during the sometimes hour-long compute times. This development then, can be viewed as responding to CONGEN users' needs as well as being an effort by the DENDRAL project to be conscientious in its resource-sharing responsibilities.

Following is a brief summary of the major users of CONGEN over the past year, as well as notes on chemists who contacted us about trial usage of the programs.

Dr. Clair Cheer, Professor of Chemistry, University of Rhode Island, Kingston, Rhode Island. Dr. Cheer is on sabbatical leave from the University of Rhode Island to the Stanford University Chemistry Department. He has, in recent work with Professor Djerassi's group, demonstrated the utility of CONGEN in the identification of (+)-Palustrol, a tricyclic sesquiterpene alcohol from the marine Xeniid **Cespitularia virdis** [57]. Dr. Cheer plans to continue his work with CONGEN once he returns to Rhode Island in December.

Dr. Jon Clardy, Professor of Chemistry, Iowa State University. Dr. Clardy read of CONGEN in an article appearing in the Journal of the American Chemical Society and contacted Professor Djerassi concerning the possibility of using the program from Iowa. He was offered GUEST access during the winter of 1975, but has not yet had an opportunity to evaluate the potentials of the program.

Dr. Douglas Dorman, Eli Lily Corp., Indianapolis, Indiana. Dr. Dorman's research involves the identification and characterization of drug related compounds by chemical and spectroscopic methods. Using primarily the NMR and C13 NMR spectra of these various compounds, Dr. Dorman has found CONGEN to be a time-saving adjunct to his structure elucidation work (see letter in Appendix B).

Dr. H.M. Fales, National Heart and Lung Institute, Bethesda, Maryland. Dr. Fales, along with Doctors Sanford Markey and Peter Roller had a joint account set up for them in April of 1975. Most of the use of this account came during late summer at which time Dr. Fales experimented with the use of CONGEN for assistance in the elucidation of the structure of a novel quinolinone, known to be tumorogenic. Although the crystal structure had been solved at the time of his usage of CONGEN, Dr. Fales felt that the program produced an abundance of useful ideas. The main problem initially faced by Dr. Fales in using CONGEN was in getting a feel for problem size and the effects of various constraint types.

Professor Kenneth Gash, California State College at Dominguez Hills. Professor Gash is a professor of chemistry who is on temporary leave to Small College, the research branch of Dominguez Hills. Dr. Gash did some of the original work, in 1965, with Professor Morton Munk, on the structure elucidation program developed at Arizona State University. Dr. Gash has been reviewing some of the problems originally done with Munk's program and has been studying input, output and constraint capabilities found in CONGEN. He has generally concluded that if system response time was better, CONGEN provides an excellent tool for the chemist to use in structure elucidation problems.

Mr. Neil A. B. Gray, King's College, Cambridge, England. Mr. Gray, following a three week visit to the Stanford chemistry department, requested copies of all the current DENDRAL programs to be sent to him in England. He is a chemist who has been working in areas related to developments in various of the DENDRAL programs, and hopes to be able to benefit from work already done at Stanford. His current interest in intelligent constraint application during structure elucidation merges well with one of the directions in which CONGEN is tending to develop. Unfortunately, Mr. Gray does not have access to an ARPANET or TYMNET node to access SUMEX-AIM directly. Therefore, all collaboration has had to be carried on by mail.

Dr. Jerrold Karliner, Ciba Geigy Corporation, Ardsley, New York. Dr. Karliner and his research group at Ciba-Geigy have become regular users of CONGEN in their day-to-day operation of a research laboratory. Dr. Karliner is a completely self-taught user of CONGEN, and has served to encourage others to request permission to use this program. A letter from Dr. Karliner, describing his usage, is attached in Appendix B.

Dr. Milton Levenberg, Abbott Laboratories, Chicago, Illinois. Dr. Levenberg has been an occasional user of CONGEN as an adjunct to his work as head of a mass spectrometry laboratory. Primary usage has been to provide assurance that the proposal of a structure for a compound on the basis of chemical and spectroscopic evidence has not overlooked other plausible possibilities.

Dr. Gino Marco, Ciba Geigy Corporation, Greensboro, North Carolina. Dr. Marco heard about CONGEN during a company seminar presented by Dr. Karliner. After a brief trial use via the GUEST mechanism, Dr. Marco requested an account for use by his group of metabolic and organic chemists. Dr. Marco's research group studies unknown insect metabolites by micro-IR and micro-NMR methods, and attempts structure elucidation based on these forms of spectroscopic analysis. Testing the utility of the program before implementing it for day to day use, Dr. Marco discovered that CONGEN could greatly narrow the alternatives of complex metabolic conjugates which had to be considered in a typical elucidation problem. They have established a leased line to the nearest TYMNET node, and expect increased CONGEN usage in the future.

Dr. David Pensak, DuPont de Nemours and Company, Wilmington, Delaware. Indirectly requested information about CONGEN through a letter written by his immediate superior to Professor Lederberg. Dr. Pensak has been offered GUEST access, and has just begun a potential collaboration with a DENDRAL group which is studying model builders and their production of reliable geometries for certain types of molecules.

Professor Manfred Wolff, University of California at San Francisco. Dr. Wolff is chairman of the Department of

Pharmacological Chemistry, and inquired as to the possibilities of accessing SUMEX-AIM and appropriate programs for a faculty which is interested in many aspects of drug design and drug action, ranging from physical chemistry to purely biological studies. He has been encouraged to use GUEST access to explore CONGEN, although he has taken no action up to the present time.

We have cases where requests for GUEST access had to be denied due to system loading considerations. We made these decisions according to the extent to which the requested use would fit within the research guidelines of SUMEX/AIM and our own stated criteria from the 1973 proposal to NIH. In one case, for instance, the use was for an individual's report on potential educational uses of CONGEN.

The following two chemists have taken advantage of CONGEN by sending appropriate data and information to Stanford.

Professor L. Minale, Laboratorio per la Chimica di Molecole di Interesse Biologico del C.N.R., Napoli, Italy. Professor Minale has been collaborating with a member of the DENDRAL staff on the solution of the structure of the cyclic diether lipids from an unusual, very thermophilic bacterium (J. C. S. Chem. Comm. 543, 1974). Application of CONGEN resulted in five final candidate structures, several of which had not previously been considered. Work is currently underway to chemically differentiate the possibilities.

Professor Kogi Nakanishi, Department of Chemistry, Columbia University. Professor Nakanishi is one of the most active and productive persons engaged in structure elucidation activities. He has developed an active interest in CONGEN and is collaborating with us on several novel problems. One of these problems has involved the structure of the active component of defense secretions of an insect (termite). Other defense secretion components are under investigation as we explore structural alternatives based on current data.

3.5 Export of GC/MS Programs to Other Sites.

There has been a demand for the GC/LRMS programs developed for data resolution and cleanup [61], and in the past several months these programs have been distributed, upon request, to five different groups. Each group was supplied with a tape, in a format appropriate to the type of computer system they were using, containing the cleanup program, as well as extensive documentation describing the program, related file structure and the required dependent utility programs.

The following research groups have already received their copies of these programs:

Professor G. Eglinton, University of Bristol, England.

Dr. Tom Elwood, Department of Chemistry, Univ. of Utah.

Dr. J. Lawless, Ames Research Center, California.

Dr. Charles Sweeley, Dept. of Biochemistry, Michigan State University.

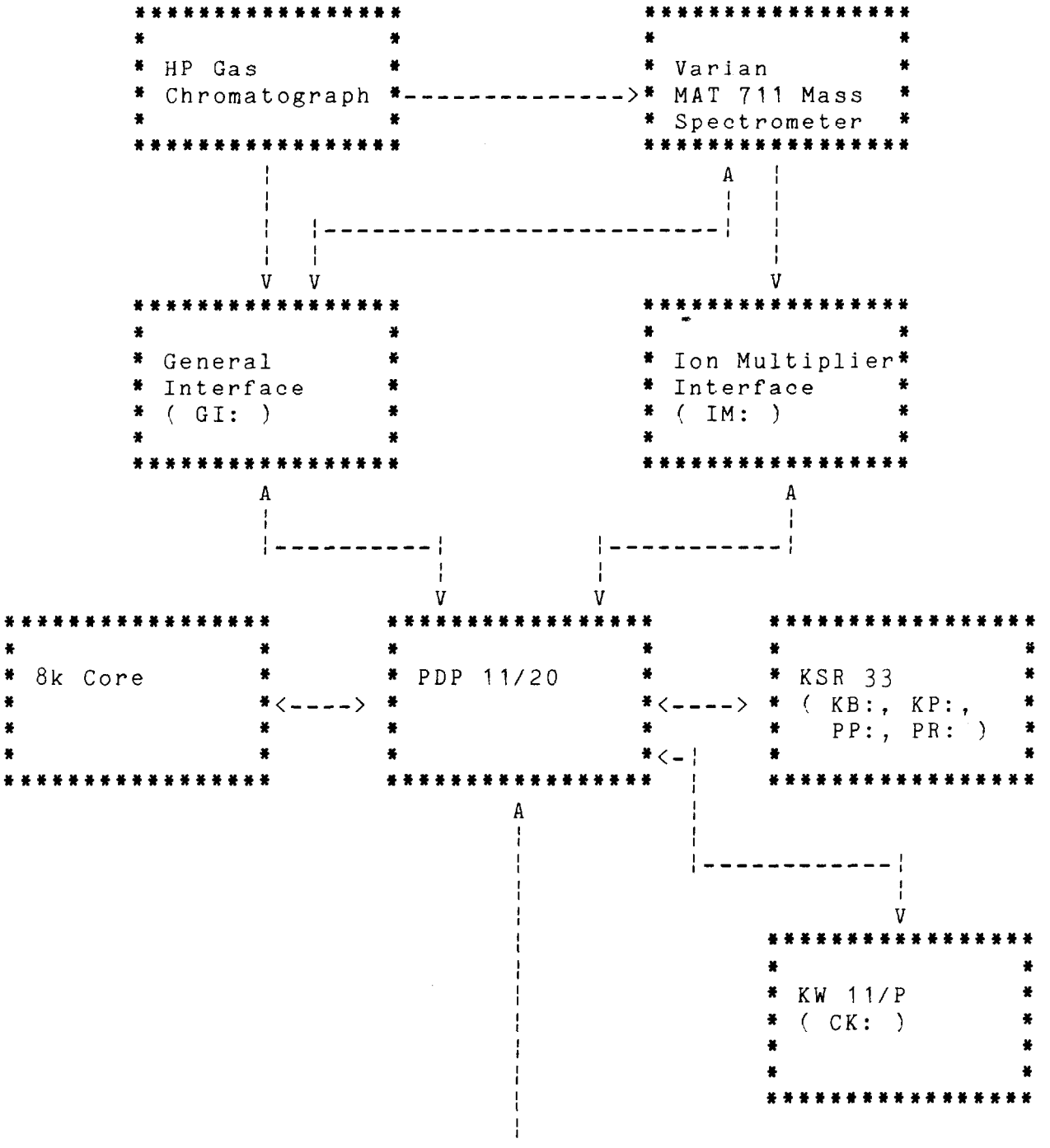
Mr. J. R. Wilcox, AEI Scientific Apparatus Inc., Elmsford, New York.

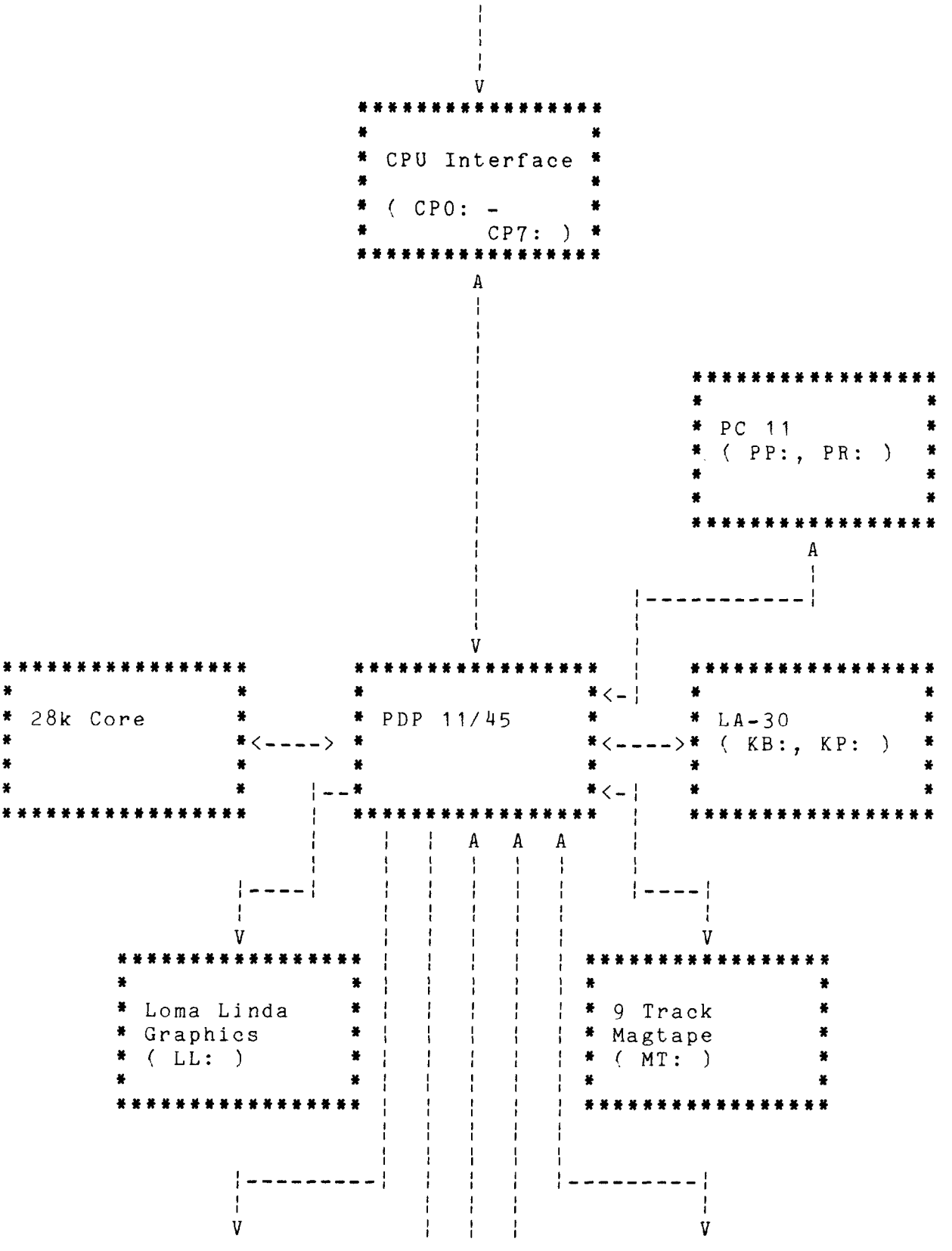
Dr. Philip Fishman, Department of Biochemistry, Washington University School of Medicine at St. Louis, Missouri has contacted us for further information concerning computer resolution of GC/MS elutants. He has been provided with the necessary information and invited to request the exportable versions of the programs.

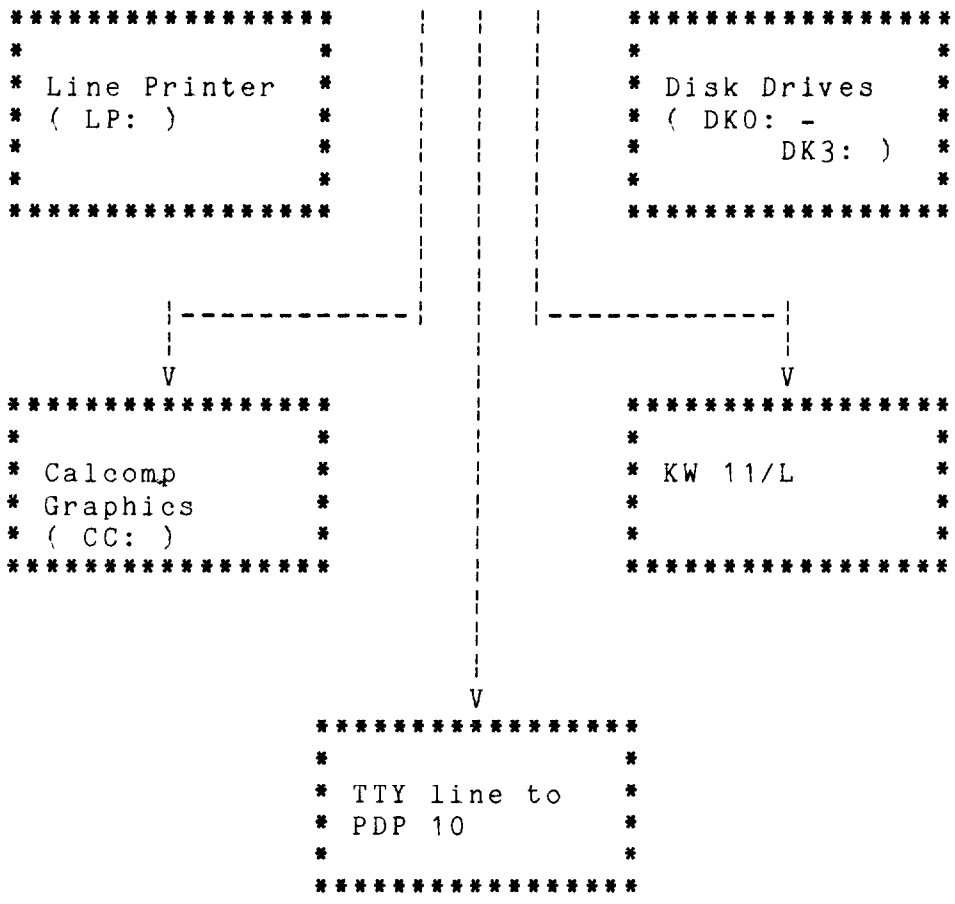
4 BIBLIOGRAPHY

See Section II-D, SUMMARY OF PUBLICATIONS, for a listing of publications by this project.

Figure 1. Current Hardware Configuration




CPU Interface
(CP0: - CP7:)
PC 11
(PP:, PR:)
28k Core
PDP 11/45
LA-30
(KB:, KP:)
Loma Linda
Graphics
(LL:)
9 Track
Magtape
(MT:)


Line Printer
(LP:)
Disk Drives
(DK0: -
DK3:)
Calcomp
Graphics
(CC:)
KW 11/L
TTY line to
PDP 10

Appendix A. Interrupt Features in a Sample CONGEN Run

```
            .
            .
  (program session has been in progress)
            .
 GENERATE
DO YOU WISH TO PRUNE WHILE GENERATING?(Y FOR YES):Y
SHALL I USE THE GLOBAL CONSTRAINT LIST?(Y FOR YES):Y
            .
            .
       (computing)
            .
            .
S
 17 structures have been generated so far
Shall I draw some?(Y for yes):Y
FROM:3
TO:3

3
    C
    =   P
C=C-C-C=H
        N
More?(Y for yes):N
Normal computation will now resume
            .
            .
27 STRUCTURES WERE GENERATED
            .
      (session continues)
            .
 IMBED
SUPERATOM NAME:PHN
DO YOU WISH TO PRUNE WHILE IMBEDDING?(Y FOR YES):N
            .
            .
     (computing)
            .
            .
I
 structure 8 of the original 19 is undergoing imbedding;
13 structures have been obtained

            .
            .
      (computing continues)
            .
            .
32 STRUCTURES WERE OBTAINED
 DRAWSOME
FROM:4
            .
            .
```

Appendix B. Letters from Collaborators

LILLY RESEARCH LABORATORIES

DIVISION OF ELI LILLY AND COMPANY • INDIANAPOLIS, INDIANA 46206 • TELEPHONE (317) 636-2211

May 6, 1976

Dr. Ray Carhart
Department of Computer Sciences
Stanford University
Stanford, California 94305

Dear Ray:

We are pleased to have an opportunity to offer our support and encouragement of your CONGEN effort.

We are using CONGEN to aid us in the solution of current structure elucidation problems. When used at an early stage, we find that the program is invaluable in suggesting the various compound types which are consistent with the extant data. In one case, for example, CONGEN generated a list of possible heteroaromatic ring systems. Such a list is particularly useful in the elucidation of the structures of pharmaceutical molecules, in that it allows us to correlate these possibilities with the physical and biological properties of a vast number of known pharmaceuticals.

In short, we have been quite pleased with our experience with CONGEN. Owing to possible security problems, we have not used the program as much as we would like. If the program were available in exportable form, I believe that usage would increase dramatically. Probably the full potential of the program will not be realized until this occurs. Even in its present form, however, CONGEN is a valuable contribution to chemistry.

Sincerely,

LILLY RESEARCH LABORATORIES

Douglas E. Dorman, Ph.D.
Physical Chemistry Research
Department MC525

CIBA-GEIGY Corporation
Ardsley, New York 10502
Telephone 914 478 3131

CIBA—GEIGY

April 19, 1976

Professor Carl Djerassi
Department of Chemistry
Stanford University
Stanford, California 94305

Dear Professor Djerassi:

Thank you for permitting us to use the CONGEN program for the past year. We have used this program only for the most demanding structure problems and therefore have not been a heavy user of the system. However, when utilized, we have found the CONGEN program to be a valuable and effective aid for structure elucidation problems.

We have used CONGEN to provide assurance that once a structure has been proposed on the basis of chemical and spectroscopic analysis that other, plausible structures have not been overlooked, thereby providing a greater confidence limit to our structural proposals. We have also utilized the program to determine possible structures when the analytical data does not provide a unique structure, and in this manner acquire additional chemical structures for consideration. Both approaches represent assets to structure determination work.

Clearly, the scope of CONGEN would be extended by making it available to other industrial chemists involved with determining structures of organic compounds. As you know, the industrial setting demands accurate results by the most rapid and economical means available. Exposing CONGEN to a wider range of industrial chemists would provide your staff with more experience with diverse structure problems and hence extend the versatility and utility of the programs. However, in order to attain more participation, the computer

system would have to be made more readily accessible, especially during peak hours. We have been fortunate in this regard since the time zone difference between Stanford and Ardsley enables us to use CONGEN early in the morning when few others are using the SUMEX programs. However, when we attempt to use the program later in the day, the system becomes fairly slow, to the point where at times we find it more economical to simply log off and resume the following morning.

We consider CONGEN as another complementary structure elucidation method at CIBA-GEIGY and look forward to its continued use in the future.

Sincerely yours,

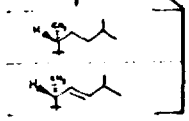
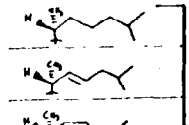
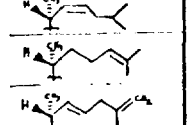
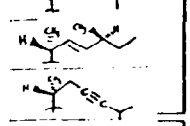
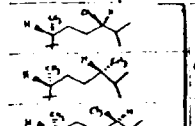
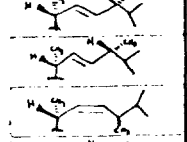
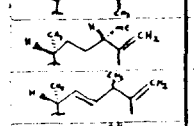
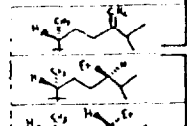
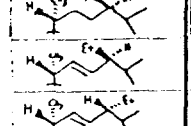
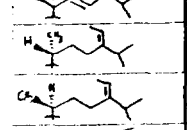
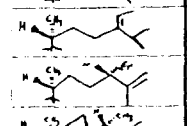
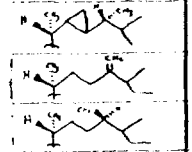
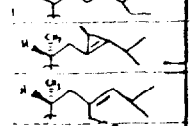
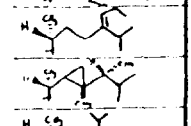
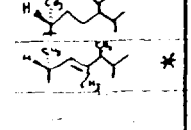
Jerrold Karliner

Jerrold Karliner Ph.D.
Group Leader
Analytical Research Department

Table I. Marine Sterol Standards

4-DEMETHYL MARINE STEROLS — Sept. 1975

Nuclei → / Side Chain ↓

Side Chain								
	A-4	A-3 (cf. M. Kobayashi)	A-1 (cf. M. Barbier) ● A-2 (cf. M. Barbier) ●				D-20	
	A-18 (133-D-19) ● A-19 (cf. S. Matsunaga) ●	A-11 (139-D-16) ● A-12 (cf. L.J. Goad) ●	A-5 (99-C-7) ● A-6	A-15 (cf. L.J. Goad) ● A-16	B-2 (133-D-18) ●	B-1	E-1 E-2 *	E-8 E-9
			A-7					
		A-13	A-8 (99-A-11) ●	A-17				
	A-20	A-14 (cf. M. Kobayashi) ●	A-9 (By M. Kobayashi) ● A-10 (cf. L.J. Goad) ●					
	B-20 C-1	B-11 (cf. M. Kobayashi, cf. B.A. Knights) ● B-12	B-3 (99-D-6) ● B-4	B-16 B-17			E-3	E-10
	C-2 (99-B-1) ● C-3	B-13 B-14 (cf. M. Kobayashi, cf. B.A. Knights) ●	B-5 B-6 (133-A-16) ●	B-18 B-19			E-4	E-11
			B-7 ● B-8 (cf. L.J. Goad) ●					
		C-14 Kallichrowa	B-9					
	C-4 (cf. A. Fattorusso) ●	B-15 (cf. L.J. Goad) ●	B-10 (99-A-12) ●				E-5	
	D-8 (99-B-17) ● D-9	C-18 C-19 (cf. M. Kobayashi, cf. B.A. Knights) ●	C-5 (99-B-16) ● C-6 (99-D-3) ●	D-4 D-5 (cf. M. Kobayashi, cf. B.A. Knights) ●			E-6	E-12
		C-20 (cf. M. Kobayashi, cf. B.A. Knights) ● D-1	C-7 (133-A-11) ● C-8 (99-B-19) ●	D-6 (cf. M. Kobayashi, cf. B.A. Knights) ● D-7			E-7	E-13
	D-10	D-2	C-9 (99-C-5) ● C-10 ?					
	D-11	D-3 (cf. L.J. Goad) ●	C-11 (cf. L.J. Goad) ● C-12 (cf. L.J. Goad) ●					
			C-13					
			C-14 C-15					
			C-16 ● C-17					
		D-13	D-12 *					
	D-19 (99-B-5) ●	D-18	D-14 (99-B-9) ● D-15					
			D-16 ● D-17					

● indicates that at least a 1 mg sample is contained in the sample box.

Shaded boxes indicate sterols which have not been found in marine sources.

indicates C-24 epimers indistinguishable by GC-MS.

] indicates a grouping of sterol side chains of identical carbon number: 7,8,9, 10, and 11.

* Note that this side chain contains 10 carbons rather than the 11 indicated by postion within bracket.

X Mass Spectrum obtained

TABLE II
Evaluation of Several Fucosterol
(Marine Algae Sterol) Mass Spectra from the
Djerassi Mass Spectral Files

```
**********************************************************

LIBRARY SEARCH REPORT FOR EXPERIMENT 21
SEARCHING   25 SPECTRA IN MARINE ON DK2

**********************************************************

( 1) SPEC #    0 RETIND      0 MOLION CANDS:     0     0     0     0     0 CR  0
                                AMPLITUDES:     0     0     0     0     0
RNK RAW AVG RETIND MOL CHEMICAL NAME                                  CR MASTER # SRC
999  87   0      0 412 (24E)-STIGMASTA-5,24(28)-DIEN-3BETA-OL          0 MARINE 18 6
729  62   0      0 412 (24E)-STIGMASTA-5,24(28)-DIEN-3BETA-OL          0 MARINE 21 6
689  51   0      0 426 (24Z)-24-PROPYLIDENECHOLEST-5-EN-3BETA-O        0 MARINE 25 6
578  44   0      0 412 (24E)-STIGMASTA-5,24(28)-DIEN-3BETA-OL          0 MARINE 19 6
544  67   0      0 412 (24E)-STIGMASTA-5,24(28)-DIEN-3BETA-OL          0 MARINE 20 6

( 2) SPEC #    0 RETIND      0 MOLION CANDS:     0     0     0     0     0 CR  0
                                AMPLITUDES:     0     0     0     0     0
RNK RAW AVG RETIND MOL CHEMICAL NAME                                  CR MASTER # SRC
999  76   0      0 412 (24E)-STIGMASTA-5,24(28)-DIEN-3BETA-OL          0 MARINE 19 6
680  51   0      0 412 (24E)-STIGMASTA-5,24(28)-DIEN-3BETA-OL          0 MARINE 21 6
574  50 999      0 412 (24E)-STIGMASTA-5,24(28)-DIEN-3BETA-OL          0 MARINE 18 6

( 3) SPEC #    0 RETIND      0 MOLION CANDS:     0     0     0     0     0 CR  0
                                AMPLITUDES:     0     0     0     0     0
RNK RAW AVG RETIND MOL CHEMICAL NAME                                  CR MASTER # SRC
999 123   0      0 412 (24E)-STIGMASTA-5,24(28)-DIEN-3BETA-OL          0 MARINE 20 6
781  61 999      0 412 (24E)-STIGMASTA-5,24(28)-DIEN-3BETA-OL          0 MARINE 18 6
694  59   0      0 412 (24E)-STIGMASTA-5,24(28)-DIEN-3BETA-OL          0 MARINE 21 6
```

II.D. SUMMARY OF PUBLICATIONS

DENDRAL PUBLICATIONS

(1) J. Lederberg, "DENDRAL-64 - A System for Computer Construction, Enumeration and Notation of Organic Molecules as Tree Structures and Cyclic Graphs", (technical reports to NASA, also available from the author and summarized in (12)). (1a) Part I. Notational algorithm for tree structures (1964) CR.57029 (1b) Part II. Topology of cyclic graphs (1965) CR.68898 (1c) Part III. Complete chemical graphs; embedding rings in trees (1969)

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